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Simulation of nanostructures excitonic spectra in an electric field

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In the most cases the modern quantum electron devices of nanoelectronics and optoelectronics are based on properties of nanostructures in an electric field. The excitonic effects are of considerable importance in the properties of these structures. It is a matter of common knowledge now and it is a reason why consideration of electric field effects on excitonic states in imperfect quantum wells is of great interest.

In general, any quantum system in electric field has continious energy spectrum, but well-known and rather simply formulas describe optical transitions only between discrete energy levels [1, 2]. The approximation of weakly interacted quantum states makes it possible to simulate in an electric field continuous electron spectrum of quantum well by Breit–Wigner resonances [3]. Therefore one can use formulas, which deal with optical transitions between quasi bound states with finite broadening. For example multiple quantum well absorption coefficient taking into account both discrete and continuous excitonic spectrum is given by

$$\alpha(\omega) = \sum_{nm} \frac{q^2 E_p \xi_m}{\pi^2 \varepsilon_0 n_\omega c m_0 \omega a_B^2 \Lambda} \left|\langle\chi_n^e|\chi_m^h\rangle\right|^2$$
$$\times \left\{ \sum_{k=1}^{\infty} \left[\hbar\Gamma_{nm}(2k-1)^{-3}\right] \left[\left(E_{nm} - \frac{R_{nm}}{(2k-1)^2} - \hbar\omega\right)^2 + (\hbar\Gamma_{nm})^2\right]^{-1} \right.$$
$$\left. + \frac{1}{4R_{nm}} \int_{E_{nm}}^{\infty} \frac{\hbar\Gamma_{nm}}{(\hbar\omega - \varepsilon)^2 + (\hbar\Gamma_{nm})^2} \frac{d\varepsilon}{1 + \exp\left(-2\pi\sqrt{\frac{\varepsilon - E_{nm}}{R_B}}\right)} \right\} \qquad (1)$$

where a_B denotes the bulk material of quantum well Bohr radius; n_ω denotes refractive index; Λ denotes the effective absorption width; $E_p = 2/m_0|\langle S|p_x|X\rangle|^2$ is related with interband matrix element of the velocity operator; $|\langle\chi_n^e|\chi_m^h\rangle|^2$ defines the probability of optical transition between n-th electron and m-th hole states; R_{nm} is a binding energy of nm exciton; $\Gamma_{nm} = \Gamma_n + \Gamma_m + \Gamma_T$, where Γ_T denotes the broadening caused by the exciton-phonon interaction; $E_{nm} = E_g + E_n + E_m$ is an energy of transition between n-th electron and m-th hole states; factor ξ_m depends on light polarization and for normal incidence equals to 1 for heavy hole and 1/3 for light hole.

The field dependence of absorption coefficient may be contained in four parameters, namely E_{nm}, Γ_{nm}, $\left|\langle\chi_n^e|\chi_m^h\rangle\right|^2$, and R_{nm}. For weakly coupled quantum wells R_{nm} depends on electric field much less then E_{nm} does [4]. Consequently we will consider only the first three parameter field dependences.

To universalize the results of our calculations all field dependences are presented in dimensionless form. We purpose to measure electric field in units of

$$F_0 = \frac{V - E_n(0)}{qL}, \qquad (2)$$

because of just the distance between energy level and top of well defines its behavior in the field. Here and then L will be the unit of coordinate, and $E_1^{\infty} = (\pi^2\hbar^2)/(2m^*L^2)$ will be the unit of energy. The origin of quasi bound states energies is taken in the center of well bottom.

Field dependences of quasi bound states energies and homogeneous broadening are presented in [3] for different dimensionless well depths. In the presented paper we pay the most attention to the field dependence of excitonic optical transition probability.

Field dependence of excitonic optical transition probability

For calculation of matrix element $\left|\langle\chi_n^e|\chi_m^h\rangle\right|^2$ as a function of electric field it is necessary to use in Eq. (2) the energy $E_n(0)$ of the most closed to continuum in the zero field state. For definition we have purposed that $\Delta E_c/\Delta E_g = 0.5$, $m_{hh} = 10m_e$, $m_{lh} = m_e$. The field dependent probability of optical transitions between n-th electron and m-th light hole states and one between n-th electron and m-th heavy hole states has only quantitative but not qualitative distinctions.

The transformation of envelope wave function symmetry in an electric field leads to existence of some maxima in field dependence of optical transition probability (see Fig. 1). The quantity of them equals to the least quantum number of the corresponding energy levels. There are n (m) maxima in these dependences if $n < m$ $(n > m)$. The absolute value of the maxima may be comparable with 1 even for “forbidden” in zero field transitions. The feature in the zero electric field of the field dependences for excitons with heavy hole is their deviation from the unity for transitions between energy levels with the same quantum numbers and nonzero probability of transitions between energy levels with even sum of their numbers. In real structures there is the feature as well for heavy hole as for light hole exciton transitions due to different tunneling of wave functions of particles with different effective mass in barriers of different height.

It’s very interesting to compare the probability of optical transitions between n-th electron and different heavy hole states in a wide range of electric field (see Fig. 2). One can see that there are some field values when symmetry-forbidden in zero field transitions are much stronger than symmetry- allowed ones. It may lead to mismatches in identification of experimental peaks. Note that in optical spectra of real structures this effect may be less visible due to the broadening of resonances.

It is possibly, that the effect discussed was the cause of observation of symmetry forbidden transitions in the room temperature photoreflectance spectrum of GaAs/GaAlAs multiple quantum well reported in Ref. [5].

Absorption spectrum of multiple quantum well in graded electric field

In real heterostructures the electric field may be uniform or graded as in optical modulator based on multiple quantum well structure replaced in i-area of $p-i-n$ diode.

In multiple quantum well (MQW) structure it is impossible to neglect by the electric field gradient inside the structure. There are some changes of optical spectra because of signal of quantum wells influenced by different values of electric field interference. In Fig. 3 the calculated by (1) spectra of GaAs/$Ga_{0.32}Al_{0.68}As$ single quantum well (dotted line) and MQW (solid line) structures are compared. The width of well is the same in both structures: $L = 9.5$ nm, barrier width is $L_B = 9.8$ nm, the quantity of quantum wells is $N = 50$. The increasing of electric field in the active region is about 25 kV/cm. The

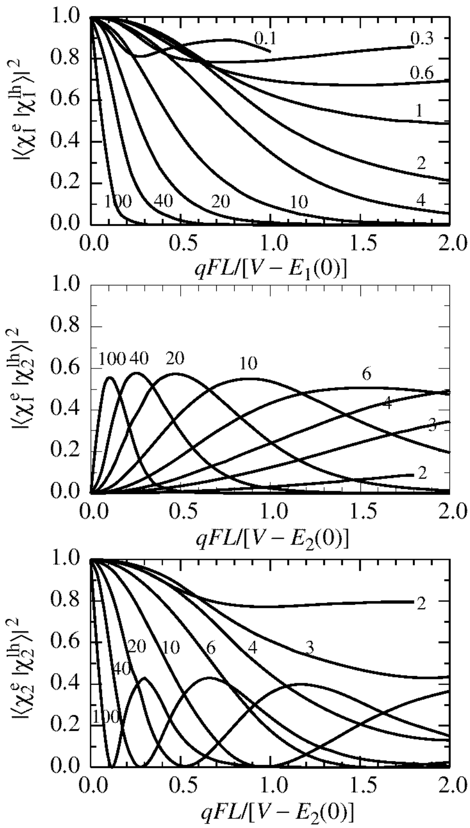

Fig. 1. The field dependence of matrix elements of excitonic optical transitions between n-th electron quasibound state and m-th light hole quasi bound state of single quantum well. Parameter notes the dimensionless quantum well depth.

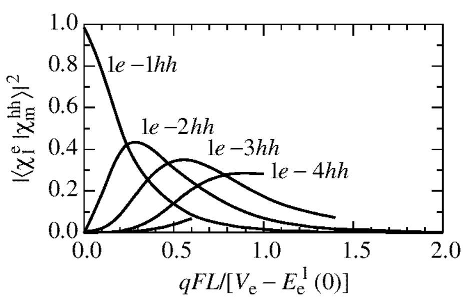

Fig. 2. The field dependence of matrix elements of excitonic optical transitions between n-th electron quasi bound state and m-th heavy hole quasi bound state of single quantum well with following parameters: $E_g = 0.985\,\mathrm{eV}$, $V_e = 120\,\mathrm{meV}$, $V_h = 80\,\mathrm{meV}$, $m_e = 0.06m_0$, $m_{hh} = 0.5m_0$, $m_{lh} = 0.07m_0$, $L = 20$ nm. The dimesionless quantum well depth is 7.6 for electrons and 42.5 for heavy holes.

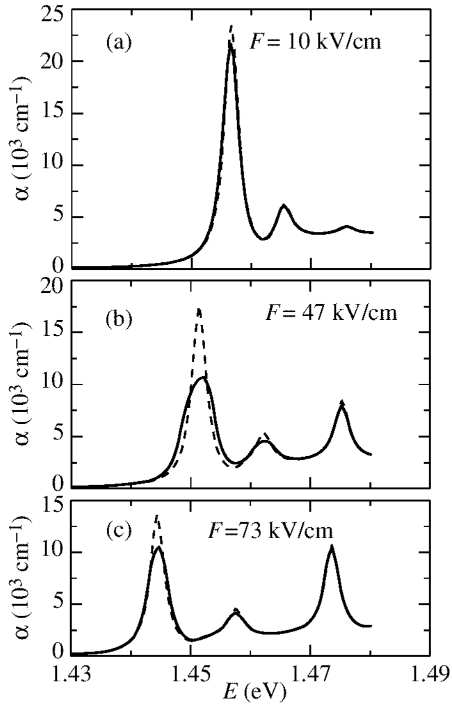

Fig. 3. The effect of gradient electric field on the absorption spectra of GaAs/$Ga_{0.32}Al_{0.68}As$ single quantum well (dotted line) and MQW (solid line) structures for different mean electric field: (a) $F = 10$ kV/cm, (b) $F = 47$ kV/cm, (c) $F = 73$ kV/cm. The width of well is the same in both structures: $L = 9.5$ nm, barrier width is $L_B = 9.8$ nm, the quantity of quantum wells is $N = 50$. The increasing of electric field in the active region is about 25 kV/cm.

comparison of calculated spectra with experimental data reported in [6] has demonstrated their good agreement.

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